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Page 1 hour per response, including the time for reviewing instructions, searching existing data sources, the collection of information. Send comments regarding this burden estimate or any other aspect of this Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Management and Budget, Paperwork Reduction Project (0704-0188) Washington, DC 20503

1. AGENCY USE ONLY (Leave blank)

2. REPORT DATE

October 10, 1992

3. REPORT TYPE AND DATES COVERED

Final 1989 - 1992

4. TITLE AND SUBTITLE

Simulation of Electronic Transport in Semiconductor
Heterolayer Devices

5. FUNDING NUMBERS

DAA-03-89-K-0037

6. AUTHOR(S)

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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

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Urbana, Illinois 618018. PERFORMING ORGANIZATION
REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

U. S. Army Research Office
P. O. Box 12211
Research Triangle Park, NC 27709-221110. SPONSORING/MONITORING
AGENCY REPORT NUMBER

ARO 26711.22-ZL

11. SUPPLEMENTARY NOTES

The view, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

A brief summary of research accomplishments during the past three years is given. Details are covered by the six submitted technical reports and twenty papers published in refereed journals.

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93-03105



14. SUBJECT TERMS

Semiconductors, Heterostructures, Devices, Electron
Transport Simulation

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION
OF REPORT

UNCLASSIFIED

18. SECURITY CLASSIFICATION
OF THIS PAGE

UNCLASSIFIED

19. SECURITY CLASSIFICATION
OF ABSTRACT

UNCLASSIFIED

20. LIMITATION OF ABSTRACT

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**SIMULATION OF ELECTRONIC TRANSPORT IN
SEMICONDUCTOR HETEROLAYER DEVICES**

FINAL REPORT

KARL HESS

October 10, 1992

U. S. ARMY RESEARCH OFFICE

**PROPOSAL NUMBER 26711EL
DAAL 03-89-K-0037**

**Beckman Institute and
Coordinated Science Laboratory
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DTIC	TAB <input type="checkbox"/>
Unannounced <input type="checkbox"/>	
Justification	
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Availability Codes	
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Progress Over the Past Three Years and ARO Sponsored Publications

Work in the three years of the grant was aimed at both improving and generalizing the full band Monte Carlo approach and at developing numerical methods to simulate transport in nanostructures. Our emphasis has been to understand transport in wide energy ranges away from the band edges. This goal can be achieved easier with the aid of computer visualization since the complexity of transport at high energies is such that visualization techniques appear indispensable. Below a brief description of the major progress is given. Details are described in 20 publications which are listed also.

- We have developed techniques of visualization in 3-dimensional geometric space and k-space with the possibility of animated sequences.

A summary of this work was described in Phys. Today [1].

In the area of Monte Carlo Transport we have:

- Developed a complete theory of impact ionization including the intracollisional field effect and collisional broadening [2-5].
- Applied Monte Carlo methods to field effect transistors and Real Space Transfer devices [6].
- Generalized the full band Monte Carlo method to include \vec{k} -dependent scattering (instead of energy dependent) and a generalized treatment of phonon scattering using a unified pseudopotential approach [8-10].

In the area of quantum transport (mesoscopic systems) we have:

- Developed numerical approaches to calculate transmission coefficients in complex nanostructures [11,12].
 - Simulated transient response in mesoscopic devices [13,14].
 - Included the effects of weak dissipation in nanostructures and mesoscopic systems [16].
 - Investigated electron-electron interactions in nanostructures by a direct numerical approach including two electrons in an exact formalism [17].
 - Developed criteria for the additivity of conductance in parallel mesoscopic channels [18,19].
- and
- Given a review of various numerical approaches that can efficiently be used to describe transport *in mesoscopic systems* [20].

ARO Sponsored Publications 1989 - 1992

- [1] K. Hess, "Supercomputer Images of Electron Device Physics," *Physics Today*, Feb. (1990).
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- [3] J. Bude, K. Hess and G. J. Iafrate, "Impact Ionization: Beyond the Golden Rule," *Proceedings of the 7th International Conference on Hot Electrons, Semicond. Sci. Technol.*, Vol. 7 pp. B506-B508, March, 1992.
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- [12] F. Sols and M. Macucci, "Circular Bands in Electron Waveguides," *Phys. Rev. B*, 41 pp. 11887-11891 (1990).
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- [15] L. F. Register, U. Ravaioli and K. Hess, "A Numerical Method for the Calculation of Transient Response in Mesoscopic Devices," *Proceedings of the NATO ASI*, D. K. Ferry, Editor, Plenum New York, pp.547, 1991.
- [16] F. Sols, "Dissipative Scattering and Transport in Mesoscopic Systems", *Proceedings of the International Symposium on Nanostructures and Mesoscopic Systems*, Santa Fe, New Mexico, 1991, Edited by W. Kirk and M. Reed, Academic Press, Inc., pp. 417-423 and F. Sols, "Scattering, Dissipation, and Transport in Mesoscopic Systems," *Annals of Physics*, Vol. 214, pp. 386-438, 1992.
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- [19] M. Macucci and K. Hess, "Conditions for the Additivity of Conductance for Parallel Mesoscopic Constrictions," *Phys. Rev. B*. accepted for publication.
- [20] M. Macucci, V. Pevzner, L. F. Register and K. Hess, "Numerical Approaches to Transport in Mesoscopic Systems," *Proceedings of the Winterschool*, Mauterndorf, Austria, February 1992, to be published.

Invited Presentations

"Monte Carlo Simulation of Electron Transport in Semiconductors at High Energies," IMACS 1st International Conference on Computational Physics, University of Colorado at Boulder, Boulder, Colorado, June 11-15, 1990.

"Approaches to Transport in Semiconductor Nanostructures," (with V. Pevzner and F. Sols) NATO Advanced Study Institute on "Granular Nanoelectronics" Il Ciocco, July 23-August 4, 1990. (see paper #11)

"Monte Carlo Simulation of Impact Ionization in Semiconductors," presented at the IBM Summer Institute on Monte Carlo Simulation on Supercomputers," Oberlech, Austria, August 13-17, 1990.

"Electronic Transport in Semiconductors at High Energy," presented at Supercomputer Symposium, University of Minnesota, Minneapolis, Minnesota, November 19-20, 1990.

"Integration Technologies of the Future: The Ultrafast, Ultrasmall, and the Ultradense," presented at the National Engineering Consortium ComForum, Phoenix, Arizona, March 14-15, 1991.

"Monte Carlo Simulations of Electronic Transport in Semiconductors at High Energies," presented at Seventh National Conference on Numerical Analysis of Semiconductor Devices and Integrated Circuits, Copper Mt., Co., April 8-12, 1991. (see paper #8)

"Numerical Approaches to Transport in Mesoscopic Systems," presented at International Conference on Mesoscopic Systems, Mauterndorf, Austria, February 24-28, 1992. (see paper #20)

"Electronic Transport in Semiconductors at High Energies," presented at NATO Workshop on Hot Electron Instabilities," Il Ciocco, September 22, 1992.

Ph.D. Thesis Finished

J. Bude Ph.D. (1992)

V. Pevzner Ph.D. (1992)